

# On the Boltzmann Equation for Weakly Nonlinear Wave Equations

Herbert Spohn

Zentrum Mathematik and Physik Department, TU München,  
Boltzmannstr. 3, D-85747 Garching, Germany

**Abstract.** We explain how the kinetic theory of L. Boltzmann is applied to weakly nonlinear wave equations.

## Introduction

Kinetic Theory is an everlasting contribution of Ludwig Boltzmann to physics. While he devised the theory to understand the dynamics of dilute gases, the method as such is much more general and has been applied with great success in many areas. A more recent example is the flow of granular media. Their defining property are inelastic collisions. Thus a natural, in fact highly informative, approach is to follow the route of kinetic theory, adjusting for the appropriate collision mechanism [1].

In the early days of kinetic theory it was a convoluted process to understand that the Boltzmann equation cannot possibly hold for every mechanical initial condition. But to set forward the proposition that the Boltzmann equation becomes exact in a particular limiting procedure, now called the Boltzmann-Grad limit [2], took almost 80 years counted from Boltzmann's 1872 paper. In this limit the sometimes painfully vague notions of "overwhelming probability" and the like acquire a definite meaning. For example, the set of exceptional initial phase points has a measure (w.r.t. the initial measure on phase space) which tends to zero in the Boltzmann-Grad limit. Grad's proposition was proved as a mathematical theorem by Lanford [3], see [4, 5] for more expanded discussions.

Given the example of low density gases, one might wonder whether similar ideas are applicable to further microscopic systems. The Landau equation for weakly interacting particles and the Vlasov equation for weak, long range forces are examples from plasma physics. After the advent of quantum mechanics, an obvious task was to also adjust kinetic theory. For electrons, satisfying Fermi-Dirac statistics, the generalization was accomplished by Nordheim [6], for the quantized wave equation (phonons) by Peierls [7], and for dilute quantum gases by Uehling and Uhlenbeck [8].

The derivation of the Boltzmann equation for interacting quantum particles is well covered in recent articles [9, 10, 11]. Here I summarize the current status for weakly nonlinear wave equations with random initial data. On the surface this problem looks simpler than weakly interacting quantum particles, since there is no need for operators,

Fock spaces, and the like. On the other hand, at least on the level of time-dependent perturbation theory, the wave equation and quantum systems have similar Feynman diagrams. In particular cases the wave diagrams are a proper subset of the set of all quantum diagrams. As a consequence the limiting kinetic equations differ only minimally. For the kinetic description a dividing line seems to be point particles versus wave equation, the latter case being much less understood because of the nonlocal interaction once the dynamics is expressed in terms of multi-point Wigner functions.

Writing down a kinetic equation always involves some modeling aspects. The available experience provides sufficient guidance as to what would constitute an acceptable kinetic equation. There is then no point in waiting for a firm microscopic derivation. Rather more urgently is to work out predictions from the kinetic equation, which by itself is a demanding endeavour. In fact, a kinetic equation to be exact in a particular limit might very well be exceptional. A prominent example are lattice Boltzmann algorithms, which are used widely to simulate flows in complicated geometries and close to reacting surfaces. For such algorithms the Boltzmann equation remains as an approximation, although a very powerful one.

To give a brief outline, in the following section we explain, what I call, the kinetic framework. Physicists tend to be more computationally oriented and the underlying statistical properties of the microscopic system are rarely spelled out in full detail. But on a conceptual level the kinetic framework is most useful and, assuming it to hold, the kinetic equation is obtained rather easily. We emphasize that the kinetic framework is not restricted to a particular model. It is a general structure, which can be used whenever a splitting into a “free” part and an appropriately small perturbation is meaningful. In Section 2 we write down the phonon Boltzmann equation in case of a quartic potential. Some of the basic properties of this equation are discussed in Section 3. Perhaps somewhat unexpected, the kinetic approach yields interesting dynamical information even for an anharmonic chain. In this light we revisit the famous Fermi-Pasta-Ulam problem.

## 1 The kinetic framework

We plan to study the scalar wave equation in three space dimensions with a cubic nonlinearity of the form

$$\frac{\partial^2}{\partial t^2}u = (\Delta - \omega_0^2)u - \sqrt{\lambda}u^3. \quad (1.1)$$

Here  $u : \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}$  is the wave field,  $\Delta$  the Laplacian, and  $\lambda > 0$ , but small. The initial data are random and of finite energy. As will be explained, the total energy is taken to be of order  $\lambda^{-3}$  and the support of  $u$  of linear extent  $\lambda^{-1}$ . To avoid the issue of ultraviolet divergencies, Eq. (1.1) is discretized spatially through the standard grid  $\mathbb{Z}^3$ . It is important to also allow for a general dispersion relation of the linear part. Physically, the discretized wave equation describes the lattice dynamics of dielectric crystals, see [12, 13, 14] for systematic expositions. In this context the scalar equation would correspond to a one-band approximation.

Fourier transform will be a convenient tool. Let  $\mathbb{T}^3 = [-\frac{1}{2}, \frac{1}{2}]^3$  be the first Brillouin zone of the lattice dual to  $\mathbb{Z}^3$ . For  $f : \mathbb{Z}^d \rightarrow \mathbb{R}$  its Fourier transform,  $\widehat{f}$ , is defined by

$$\widehat{f}(k) = \sum_{x \in \mathbb{Z}^3} e^{-i2\pi k \cdot x} f_x. \quad (1.2)$$

Here  $k \in \mathbb{T}^3$  and  $\widehat{f}$  extends periodically to a function on  $\mathbb{R}^3$ . The inverse Fourier transform is given by

$$f_x = \int_{\mathbb{T}^3} dk e^{i2\pi k \cdot x} \widehat{f}(k). \quad (1.3)$$

For  $x \in \mathbb{Z}^3$  the displacement away from  $x$  is denoted by  $q_x \in \mathbb{R}$  and the corresponding momentum by  $p_x \in \mathbb{R}$ . In the harmonic approximation the interaction potential is

$$U_{\text{harm}}(q) = \frac{1}{2} \sum_{x, y \in \mathbb{Z}^3} \alpha(x - y) q_x q_y. \quad (1.4)$$

The elastic constants  $\alpha(x)$  satisfy

$$\alpha(x) = \alpha(-x) \quad \text{and} \quad |\alpha(x)| \leq \gamma_0 e^{-\gamma_1 |x|} \quad (1.5)$$

for suitable  $\gamma_0, \gamma_1 > 0$ . Mechanical stability requires

$$\widehat{\alpha}(k) \geq 0. \quad (1.6)$$

In fact, we assume  $\widehat{\alpha}(k) > 0$  for  $k \neq 0$ . The case  $\widehat{\alpha}(k) \simeq k^2$  for small  $k$  is referred to as ‘acoustical’ while  $\widehat{\alpha}(0) > 0$  is ‘optical’. The dispersion relation of the harmonic part is

$$\omega(k) = \sqrt{\widehat{\alpha}(k)}. \quad (1.7)$$

Following (1.1) as a concrete example, we consider a quartic on-site potential. Then the full hamiltonian of the lattice dynamics is given by

$$H = \frac{1}{2} \sum_{x \in \mathbb{Z}^3} p_x^2 + \frac{1}{2} \sum_{x, y \in \mathbb{Z}^3} \alpha(x - y) q_x q_y + \frac{1}{4} \sqrt{\lambda} \sum_{x \in \mathbb{Z}^3} q_x^4. \quad (1.8)$$

The harmonic part of  $H$  will be denoted by  $H_{\text{ha}}$ ,  $H = H_{\text{ha}} + \sqrt{\lambda} V$ . In a sense to be explained below,  $\sqrt{\lambda} V$  is a “small” perturbation of  $H_{\text{ha}}$ .

We concatenate  $q_x$  and  $p_x$  into a single complex-valued field  $a(k)$  as

$$a(k) = \frac{1}{\sqrt{2}} \left( \sqrt{\omega(k)} \widehat{q}(k) + i \frac{1}{\sqrt{\omega(k)}} \widehat{p}(k) \right) \quad (1.9)$$

with the inverse

$$\widehat{q}(k) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{\omega(k)}} (a(k) + a(-k)^*), \quad \widehat{p}(k) = \frac{i}{\sqrt{2}} \sqrt{\omega(k)} (-a(k) + a(-k)^*). \quad (1.10)$$

Then the hamiltonian reads

$$H = H_{\text{ha}} + \sqrt{\lambda} V, \quad H_{\text{ha}} = \int_{\mathbb{T}^3} dk \omega(k) a(k)^* a(k), \quad (1.11)$$

$$V = \frac{1}{4} \int_{\mathbb{T}^{12}} dk_1 dk_2 dk_3 dk_4 \delta(k_1 + k_2 + k_3 + k_4) \\ \times \prod_{j=1}^4 (2\omega(k_j))^{-1/2} (a(k_j) + a(-k_j)^*). \quad (1.12)$$

Hence the equations of motion for the  $a$ -field are

$$\frac{\partial}{\partial t} a(k, t) = -i\omega(k) a(k, t) - i\sqrt{\lambda} \int_{\mathbb{T}^9} dk_1 dk_2 dk_3 \delta(k - k_1 - k_2 - k_3) \\ \times (2\omega(k))^{-1/2} \prod_{j=1}^3 (2\omega(k_j))^{-1/2} (a(k_j, t) + a(-k_j, t)^*). \quad (1.13)$$

In particular for  $\lambda = 0$ ,

$$a(k, t) = e^{-i\omega(k)t} a(k). \quad (1.14)$$

Let us now briefly recall the case of dilute gases. The central quantity is the Boltzmann  $f$ -function, which is the number density on one-particle phase space  $\mathbb{R}^3 \times \mathbb{R}^3$ . It changes in time by the free motion of particles and through pair collisions,

$$\frac{\partial}{\partial t} f_t + v \cdot \nabla_r f_t = C(f_t, f_t). \quad (1.15)$$

We do not write out the collision operator explicitly but note that it is bilinear in  $f_t$  and strictly local in the space-variable  $r$ , since on the kinetic scale particles collide at the same point. At low density the full particle statistics is close to Poisson, jointly in positions and velocities, with an intensity given again by the  $f$ -function. This double meaning of the  $f$ -function is a source of conceptual confusion. In the Stoßzahlansatz one assumes independent incoming velocities, thus the second meaning of  $f$ , while the predictions of kinetic theory are based on a law of large numbers, thus the first meaning of  $f$ . The Poisson statistics appears naturally through the good statistical mixing properties of the collisionless dynamics. In fact, at infinite volume, these are the only translation invariant measures, which are invariant under the collisionless dynamics and which have a finite number, energy, and entropy per unit volume [15].

For wave equations the Poisson measure will be substituted by a Gaussian measure, constrained to be locally invariant under the dynamics generated by  $H_{\text{ha}}$ . In the *spatially homogeneous* case, imposing time-stationarity and using the explicit solution (1.14) for  $\lambda = 0$ , the  $\{a(k), k \in \mathbb{T}^3\}$  are then jointly Gaussian with mean zero and covariance

$$\langle a(k)^* a(k') \rangle = W(k) \delta(k - k'), \quad (1.16)$$

$$\langle a(k)^* a(k')^* \rangle = 0, \quad \langle a(k) a(k') \rangle = 0, \quad (1.17)$$

defining the power spectrum  $W(k)$ . Clearly,  $W(k) \geq 0$ .

For the *spatially inhomogeneous* case the construction is slightly more elaborate. Since the anharmonic potential is of order  $\sqrt{\lambda}$ , the mean free path for phonons is of order  $\lambda^{-1}$ . This is the scale on which spatial inhomogeneities have to be imposed. Local stationarity still implies mean zero and (1.17). For the covariance (1.16) we first prescribe the limiting local power spectrum  $W : \mathbb{R}^3 \times \mathbb{T}^3 \rightarrow \mathbb{R}$  with  $W \geq 0$  and a rapid decay in position space. In analogy to the semiclassical limit of the Schrödinger equation we refer to  $W$  as Wigner function. A *locally stationary* Gaussian measure, denoted by  $\langle \cdot \rangle^{G,\lambda}$ , is in fact a scale of probability measures depending on  $\lambda$ . For each  $\lambda$  the measure  $\langle \cdot \rangle^{G,\lambda}$  is Gaussian with

$$\langle a(k) \rangle^{G,\lambda} = 0, \quad \langle a(k) a(k') \rangle^{G,\lambda} = 0. \quad (1.18)$$

Following Wigner the local power spectrum of the  $a$ -field is defined through

$$P^1(x, k) = 2^{-3} \int_{(2\mathbb{T})^3} d\eta e^{i2\pi x \cdot \eta} a(k - \eta/2)^* a(k + \eta/2). \quad (1.19)$$

We rescale the lattice to have lattice spacing  $\lambda$  through the substitution  $x = \lambda^{-1}y$ ,  $y \in (\lambda\mathbb{Z}/2)^3$ , and obtain the rescaled local power spectrum

$$P^\lambda(y, k) = (\lambda/2)^3 \int_{(2\mathbb{T}/\lambda)^3} d\eta e^{i2\pi y \cdot \eta} a(k - \lambda\eta/2)^* a(k + \lambda\eta/2). \quad (1.20)$$

$P^\lambda$  is a random field. By definition, its average is the one-particle Wigner function,

$$W_1^\lambda(y, k) = \langle P^\lambda(y, k) \rangle^{G,\lambda} \quad (1.21)$$

and its variance the two-particle Wigner function,

$$W_2^\lambda(y_1, k_1, y_2, k_2) = \langle P^\lambda(y_1, k_1) P^\lambda(y_2, k_2) \rangle^{G,\lambda}. \quad (1.22)$$

With  $\lfloor \cdot \rfloor_\lambda$  denoting modulo  $\lambda$ , the scale of Gaussian measures  $\langle \cdot \rangle^{G,\lambda}$  is assumed to satisfy the pointwise limit

$$\lim_{\lambda \rightarrow 0} W^\lambda(\lfloor r \rfloor_\lambda, k) = W(r, k). \quad (1.23)$$

Furthermore one has to require a law of large numbers for the power spectrum  $P^\lambda$  which can be expressed in the form

$$\lim_{\lambda \rightarrow 0} W_2^\lambda(\lfloor r_1 \rfloor_\lambda, k_1, \lfloor r_2 \rfloor_\lambda, k_2) = W(r_1, k_1) W(r_2, k_2) \quad (1.24)$$

for  $r_1 \neq r_2$ .

In general, the assumption of strict Gaussianity is too strong. Because of the anharmonicity, unavoidably there will be small errors. To allow for them we call an arbitrary sequence of probability measures,  $\langle \cdot \rangle^\lambda$ , *locally stationary*, if the Gaussian property is gained

only in the limit  $\lambda \rightarrow 0$ . More precisely, for our model we may assume that all odd moments of  $\langle \cdot \rangle^\lambda$  vanish, since this property is propagated in time. For the second moments  $\langle a(k)a(k') \rangle^\lambda$ ,  $\langle a(k)^*a(k') \rangle^\lambda$  we form the rescaled one-particle Wigner function as in (1.20), (1.21). The rescaled Wigner function for  $\langle a(k)a(k') \rangle^\lambda$  is assumed to vanish as  $\lambda \rightarrow 0$ , while the rescaled Wigner function for  $\langle a(k)^*a(k') \rangle^\lambda$  satisfies (1.23). (1.24) is imposed correspondingly. In addition we require that the sequence of local measures, close to  $\lambda^{-1}r$  [lattice units], converges to a Gaussian measure with covariance (1.16), (1.17) and  $W(k)$  replaced by  $W(r, k)$ .

From (1.23) we infer that for a locally stationary measure it holds

$$\langle H_{\text{ha}} \rangle^\lambda = \int_{\mathbb{T}^3} dk \omega(k) \langle a(k)^*a(k) \rangle^\lambda = O(\lambda^{-3}). \quad (1.25)$$

The harmonic energy is extensive. On the other hand the average anharmonic potential satisfies  $\sqrt{\lambda} \langle V \rangle^\lambda = \sqrt{\lambda} O(\lambda^{-3})$ , which is small compared to  $\langle H_{\text{ha}} \rangle^\lambda$ .

Our real goal is to understand the time evolution in the limit of small  $\lambda$ . We impose the initial measure to be Gaussian and locally stationary. As a simple, but useful first step we set  $V = 0$  and, for a short intermediate stretch only, consider the linear dynamics generated by  $H_{\text{ha}}$ . By linearity this dynamics preserves the Gaussian property. Since the initial state has a slow variation on the scale  $\lambda^{-1}$ , the limit  $\lambda \rightarrow 0$  for the one-particle Wigner function is a particular case of the semiclassical limit for a linear wave equation. Thus the appropriate time scale is also of order  $\lambda^{-1}$  and on that scale

$$\lim_{\lambda \rightarrow 0} W^\lambda(\lfloor r \rfloor_\lambda, k, \lambda^{-1}t) = W(r, k, t). \quad (1.26)$$

(On the left hand side  $\lambda^{-1}t$  is the time in microscopic units, the units of (1.13), while on the right hand side  $t$  refers to kinetic times, the units for (1.15)). The limit Wigner function is governed by the transport equation

$$\frac{\partial}{\partial t} W(r, k, t) + \frac{1}{2\pi} \nabla_k \omega(k) \cdot \nabla_r W(r, k, t) = 0, \quad (1.27)$$

which corresponds to the free motion of fictitious particles, the phonons, with kinetic energy  $\omega$ . Of course, (1.27) has to be solved with the initial condition  $W(r, k, 0) = W(r, k)$ .

We refer to [16, 17] for a complete coverage of the semiclassical limit for lattice dynamics with an arbitrary unit cell. Random initial data are studied in [18], where only rather mild mixing conditions on the initial measure  $\langle \cdot \rangle^\lambda$  are imposed. Let  $\langle \cdot \rangle_t^\lambda$  be the measure at time  $t$  as evolved according to the dynamics generated by  $H_{\text{ha}}$ . It is proved that for any  $t > 0$  the sequence of measures  $\langle \cdot \rangle_{\lambda^{-1}t}^\lambda$  is locally stationary with a Wigner function satisfying the transport equation (1.27). In this sense local stationarity is dynamically generated. Such results require, as does the kinetic limit, that phonons propagate with nonzero velocity. To say one has to demand that  $\nabla_k \omega \neq 0$  a.s.. By our assumption,  $\omega^2$  is real analytic on  $\mathbb{T}^3$  and one only has to exclude the case  $\omega = \text{const.}$ . Nevertheless, since momentum space is  $\mathbb{T}^3$ , there will always be submanifolds where  $\nabla_k \omega = 0$ , which sets an extra technical difficulty.

We return to the case of interest, namely adding the anharmonicity  $\sqrt{\lambda}V$ . Then, if as before the initial measure is required to be Gaussian and locally stationary, the time-evolved measure  $\langle \cdot \rangle_t^{G,\lambda}$  is no longer Gaussian. On the other hand, the linear dynamics does not tolerate deviations from Gaussianity, as demonstrated in [18], and the strength of the anharmonicity is taken to be small. Thus the family  $\langle \cdot \rangle_{\lambda^{-1}t}^{G,\lambda}$  is still locally stationary. Of course now  $W(k)$  depends on  $r$  and  $t$  [kinetic scale]. The precise strength of the anharmonic on-site potential is adjusted such that its effect is of order 1 for the scale on which (1.27) holds. More physically speaking, the interaction strength is such that the phonon mean free path is of order  $\lambda^{-1}$  [lattice units]. Thus one expects the limit (1.26) still to be valid. Only the transport equation picks up a term resulting from the collisions between phonons.

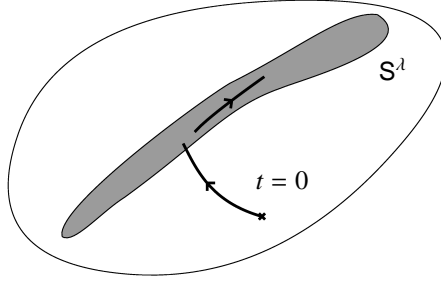


Figure 1. Time evolution of a probability measure under kinetic scaling.

We summarize the kinetic framework by means of a somewhat schematic diagram. The encircled set is supposed to represent the set of “all” probability measures for the random field  $a(k)$ . We fix the interaction strength as  $0 < \lambda \ll 1$ . The manifold-like set denoted by  $S^\lambda$  is the set of all locally stationary measures up to some  $\lambda$ -dependent scale of precision. The hamiltonian dynamics generates a flow on the space of measures. The set  $S^\lambda$  is attractive, in the sense that fairly rapidly, times of order 1, the measure will be close to  $S^\lambda$ . On  $S^\lambda$  the time evolution is slow with changes on the kinetic scale  $O(\lambda^{-1})$  and the defining Wigner function is governed by a kinetic equation. For  $t \gg \lambda^{-1}$  further dynamical phenomena set in which cannot be captured through the kinetic framework.

## 2 The Boltzmann equation

The kinetic framework provides us with a tool for an educated guess on the form of the collision operator. An important check will be that the resulting equation has the physically correct stationary solutions and satisfies an  $H$ -theorem for the total entropy, respectively a local semi-conservation law with a positive entropy production.

A more demanding issue is to support the educated guess by mathematical arguments which establish the assumed existence of limits and local stationarity.

Let  $\langle \cdot \rangle_t^{G,\lambda} = \langle \cdot \rangle_t$  denote the measure at time  $t$  under the dynamics generated by  $H$  with  $\langle \cdot \rangle_0 = \langle \cdot \rangle^{G,\lambda}$ . The two-point function satisfies

$$\frac{d}{dt} \langle a(p)^* a(q) \rangle_t = i(\omega(p) - \omega(q)) \langle a(p)^* a(q) \rangle_t + \sqrt{\lambda} F(q, p, t). \quad (2.1)$$

$F$  is cubic in the  $a$ -field. We integrate (1.13) in time, symbolically

$$a(t) = e^{-i\omega t} a + \sqrt{\lambda} \int_0^t e^{-i\omega(t-s)} a(s)^3, \quad (2.2)$$

and insert (2.2) in the expression for  $F$ . There are then cubic terms, proportional to  $\sqrt{\lambda}$ , which vanish upon averaging, and sextic terms, proportional to  $\lambda$ . At this point we use, as argued, that locally the measure is approximately Gaussian and factorize the 6-point function according to the Gaussian rule for moments. We also rescale space-time by  $\lambda^{-1}$  and switch to Wigner function coordinates. In this form one can take the limit  $\lambda \rightarrow 0$ . The first term on the right of (2.1) yields the free flow while  $\sqrt{\lambda} F$  results in the collision operator with a cubic nonlinearity.

Details of such computations can be found in [9, 19]. Here we only quote the result, which is the Boltzmann equation

$$\frac{\partial}{\partial t} W(r, k, t) + \frac{1}{2\pi} \nabla_k \omega(k) \cdot \nabla_r W(r, k, t) = C(W(r, t))(k). \quad (2.3)$$

The collision operator is local in  $r, t$ , which our notation is supposed to indicate.  $C$  is a nonlinear functional of  $k \mapsto W(r, k, t)$  at fixed  $r, t$ . For the quartic on-site potential,  $C$  is cubic and defined through

$$\begin{aligned} C(W)(k) = 12\pi \sum_{\sigma_1, \sigma_2, \sigma_3 = \pm 1} \int_{\mathbb{T}^9} dk_1 dk_2 dk_3 (16\omega\omega_1\omega_2\omega_3)^{-1} \\ \times \delta(k + \sigma_1 k_1 + \sigma_2 k_2 + \sigma_3 k_3) \delta(\omega + \sigma_1 \omega_1 + \sigma_2 \omega_2 + \sigma_3 \omega_3) \\ \times (W_1 W_2 W_3 + W(\sigma_1 W_2 W_3 + W_1 \sigma_2 W_3 + W_1 W_2 \sigma_3)), \end{aligned} \quad (2.4)$$

where we use the shorthand  $W_j = W(k_j)$ ,  $\omega_j = \omega(k_j)$ ,  $j = 1, 2, 3$ . The term proportional to  $W$  is the loss term. It has no definite sign. On the other hand the gain term  $W_1 W_2 W_3$  is always positive, ensuring that the positivity of the initial Wigner function is propagated in time.

As a historical parenthesis we remark that in his seminal paper Peierls uses a very different reasoning. The current method goes back to the mid-fifties where Green's function techniques were developed systematically along the lines set forth by Quantum Field Theory. The textbook expositions of the phonon Boltzmann equation are not so satisfactory, at least in solid state physics. For the quantized theory Fermi's golden rule is applied in a spatially homogeneous, discrete mode context. While this gives the correct collision operator, the 'why' remains obscure. Classical lattice dynamics is conceived only as a  $\hbar \rightarrow 0$  limit of the quantum theory. The situation is more favorable in wave turbulence, where the starting point is a weakly nonlinear system of wave equations in hamiltonian



form [20]. Statistical properties are accessible and the validity of Gaussian statistics is an important issue [21, 22].

At present, we are very far away from a complete mathematical proof of the existence of the limit in Eq. (1.26) together with the property that the limiting Wigner function is the solution to (2.3), (2.4) with initial conditions  $W(r, k, 0) = W(r, k)$ . Apparently, the only available technique is to expand with respect to  $\sqrt{\lambda}V$  into a time-dependent perturbation series. Each term of the series can be represented symbolically as a Feynman diagram, which represents an oscillatory integral. In the limit  $\lambda \rightarrow 0$  most diagrams vanish (subleading diagrams) and a few do not vanish (leading diagrams). The sum over all leading diagrams yields the time-dependent perturbation series of the Boltzmann equation, where the free flow is integrated and the collision term is regarded as perturbation. The conjectured division into leading and subleading diagrams is explained in [23].

The program outlined has been carried out only fragmentarily. The first order, proportional to  $\sqrt{\lambda}$ , vanishes. To second order one expects the limit

$$\int_0^t ds e^{L(t-s)} C(e^{Ls} W), \quad (2.5)$$

where  $(e^{Lt} W)(r, k) = W(r - (2\pi)^{-1} \nabla_k \omega(k)t, k)$ . While such limit could be established at the level of generality discussed here, even this point has not been accomplished. Closest to the goal comes the very careful analysis of Ho and Landau [24], who study the same problem for a weakly interacting Fermi liquid on  $\mathbb{Z}^3$  with nearest neighbor hopping and obtain the analogue of (2.5). Benedetto *et al.* [25, 26] consider a weakly interacting quantum fluid in  $\mathbb{R}^3$  with the usual kinetic energy  $p^2/2m$ . In our context this would correspond to the nonlinear Schrödinger equation,  $m = 1$ ,

$$i \frac{\partial}{\partial t} \psi(x, t) = \left( -\frac{1}{2} \Delta_x + \sqrt{\lambda} V_\psi(x, t) \right) \psi(x, t) \quad (2.6)$$

with the effective potential

$$V_\psi(x, t) = \int_{\mathbb{R}^3} dy \vartheta(x - y) |\psi(y, t)|^2. \quad (2.7)$$

$\vartheta$  smoothens the interaction on a microscopic scale. The role of the  $a$ -field is taken over by the Fourier transform  $\widehat{\psi}$ . The Wigner function  $W^\lambda(t)$  is precisely the standard Wigner function for the Schrödinger equation at time  $\lambda^{-1}t$  averaged over the initial Gaussian distribution of the  $\psi$ -field. The Boltzmann equation for the nonlinear Schrödinger equation (2.6) has the same overall structure as (2.3), (2.4). More precisely, now  $k \in \mathbb{R}^3$  and

$$\frac{\partial}{\partial t} W(r, k, t) + k \cdot \nabla_r W(r, k, t) = C_{\text{NS}}(W(r, t))(k) \quad (2.8)$$

with the collision operator

$$\begin{aligned} C_{\text{NS}}(W)(k_1) &= 12\pi \int_{\mathbb{R}^9} dk_2 dk_3 dk_4 |\widehat{\vartheta}(k_1 - k_2)|^2 2\delta(k_1^2 + k_2^2 - k_3^2 - k_4^2) \\ &\quad \times \delta(k_1 + k_2 - k_3 - k_4) (W_2 W_3 W_4 - W_1 (W_2 W_3 + W_2 W_4 - W_3 W_4)). \end{aligned} \quad (2.9)$$

The Feynman diagrams of the nonlinear Schrödinger equation are a proper subset of those investigated in [25]. Using their result, one concludes that in the limit  $\lambda \rightarrow 0$  the second order expansion term is given by (2.5) with the appropriate adjustments for  $L$  and  $C$ .

### 3 Stationary solutions, entropy production

For dilute gases the  $f$ -function derived from the thermal equilibrium distribution of the  $N$ -particle system is a stationary solution of the kinetic equation. If one identifies the entropy with the logarithm of phase space volume associated to some given  $f$ -function on one-particle phase space, then the entropy functional turns out to be

$$S(f) = - \int dv f(v) \log f(v), \quad (3.1)$$

in units where Boltzmann's constant  $k_B = 1$ .  $S(f)$  is increasing in time and constant if and only if  $f$  is Maxwellian (at least in the spatially homogeneous case). Thus the reader may wonder whether the phonon Boltzmann equation has similar properties.

To determine the collision rule for phonons, one has to solve the conservation laws of energy and momentum, see Eq (2.4). For pair collisions, i.e.  $\sum_{j=1}^3 \sigma_j = -1$ , this amounts to

$$\omega(k_1) + \omega(k_2) = \omega(k_3) + \omega(k_1 + k_2 - k_3) \quad (3.2)$$

and for three phonons mergers to

$$\omega(k_1) + \omega(k_2) + \omega(k_3) = \omega(k_1 + k_2 + k_3), \quad (3.3)$$

where both equations implicitly define  $k_3 = k_3(k_1, k_2)$ .  $k_4$  is obtained from momentum conservation as  $k_4 = k_1 + k_2 - k_3 \bmod 1$ , resp.  $k_4 = k_1 + k_2 + k_3 \bmod 1$ . Mostly one has to work with this implicit definition and only in very exceptional cases an explicit collision formula is available. An instructive example is the case one space dimension. Mechanical particles would merely exchange labels and the Boltzmann collision operator vanishes. On the other hand, for phonons in one dimension with an  $\omega$  derived from nearest neighbor couplings, (3.2) has a nondegenerate solution, thus providing real phonon collisions [27, 28]. In principle, it may happen that the energy-momentum conservation laws have no solution at all. Then the collision term vanishes. In case of several solutions one has to sum over all of them. Note that in (2.4) energy conservation cannot be satisfied for the term with  $\sigma_j = 1$ ,  $j = 1, 2, 3$ . This term had been added only to have a more symmetric looking expression. A further instructive example are nearest neighbor couplings, for which the dispersion relation reads

$$\omega(k) = \left( \omega_0^2 + 2 \sum_{j=1}^3 (1 - \cos(2\pi k^j)) \right)^{1/2}, \quad k = (k^1, k^2, k^3) \in \mathbb{T}^3. \quad (3.4)$$

Then (3.3) has no solution and collision processes where three phonons merge into one, and their time reversal, are forbidden. As for dilute gases, there are only number conserving pair collisions. Such a property is stable under small perturbations of  $\omega$ . It also holds for the nonlinear wave equation (1.1) for which  $\omega(k) = |k|$ ,  $k \in \mathbb{R}^3$ .

The equilibrium measure for the harmonic part is the Gaussian  $Z^{-1} \exp[-\beta H_{\text{har}}]$  with  $Z$  the normalizing partition function and  $\beta$  the inverse temperature,  $\beta > 0$ . The anharmonic potential can be neglected in the kinetic limit. The corresponding Wigner function,  $W_\beta$ , is given by

$$W_\beta(k) = \frac{1}{\beta \omega(k)}, \quad (3.5)$$

in the limit of an infinitely extended lattice, compare with (1.16). Using (2.4), it follows that

$$\begin{aligned} C(W_\beta)(k) &= \frac{3\pi}{4} \sum_{\sigma_1, \sigma_2, \sigma_3 = \pm 1} \int_{\mathbb{T}^3} dk_1 dk_2 dk_3 (\omega \omega_1 \omega_2 \omega_3)^{-1} \delta(\omega + \sigma_1 \omega_1 + \sigma_2 \omega_2 + \sigma_3 \omega_3) \\ &\quad \times \delta(k + \sigma_1 k_1 + \sigma_2 k_2 + \sigma_3 k_3) \beta^{-3} (\omega \omega_1 \omega_2 \omega_3)^{-1} (\omega + \sigma_1 \omega_1 + \sigma_2 \omega_2 + \sigma_3 \omega_3) \\ &= 0, \end{aligned} \quad (3.6)$$

as expected. The issue whether there are further stationary solutions will be discussed below.

Following Boltzmann, to define the entropy one first has to identify a family of macroscopic observables. If for simplicity, and in fact for the remainder of this section, we restrict ourselves to the spatially homogeneous situation, then in spirit the macrovariables are the phonon numbers  $a(k)^* a(k)$ ,  $k \in \mathbb{T}^3$ . To be more precise one has to employ the limit procedure of Boltzmann, the only difference being that here we have to take into account the harmonic couplings. We partition the torus  $\mathbb{T}^3$  into cubes  $\Delta_j$  of side length  $\delta$ ,  $j = 1, \dots, M^3$ ,  $\delta M = 1$ . We consider a finite lattice volume,  $\ell^3$ , which is equivalent to discretizing the torus  $\mathbb{T}^3$  to  $(\mathbb{T}_\ell)^3$  with grid spacing  $\ell^{-1}$ . The proper macrovariables are then

$$H_j = \sum_{k \in \Delta_j \cap (\mathbb{T}_\ell)^3} a(k)^* a(k), \quad j = 1, \dots, M^3. \quad (3.7)$$

For a given Wigner function  $W$  the cell in phase space at precision  $\ell^3 \varepsilon$  is defined by the conditions

$$\{(q, p) \in (\mathbb{R}^2)^{\ell^3} \mid \ell^3(e_j - \varepsilon) \leq H_j(q, p) \leq \ell^3(e_j + \varepsilon), \quad j = 1, \dots, M^3\} \quad (3.8)$$

with

$$e_j = \delta^3 \int_{\Delta_j} dk W(k). \quad (3.9)$$

The entropy  $S(W)$  of  $W$  is defined as  $\ell^{-3}$  times the logarithm of the Lebesgue measure of the set in (3.8) upon taking limits in the following order:  $\ell \rightarrow \infty$ ,  $\varepsilon \rightarrow 0$ ,  $\delta \rightarrow 0$ . The net result is

$$S(W) = \int_{\mathbb{T}^3} dk \log W(k), \quad (3.10)$$

up to a constant independent of  $W$ .

Before computing the rate of change of the entropy let us introduce the notion of a collisional invariant. This is a function  $\psi : \mathbb{T}^3 \rightarrow \mathbb{R}$  which satisfies either one of the following functional equations.

(i) (*pair collisions*)

$$\psi(k_1) + \psi(k_2) = \psi(k_3) + \psi(k_1 + k_2 - k_3) \quad (3.11)$$

on the set  $\{(k_1, k_2, k_3) \in \mathbb{T}^9 \mid \omega(k_1) + \omega(k_2) = \omega(k_3) + \omega(k_1 + k_2 - k_3)\}$ .

(ii) (*three phonons merger*)

$$\psi(k_1) + \psi(k_2) + \psi(k_3) = \psi(k_1 + k_2 + k_3) \quad (3.12)$$

on the set  $\{(k_1, k_2, k_3) \in \mathbb{T}^3 \mid \omega(k_1) + \omega(k_2) + \omega(k_3) = \omega(k_1 + k_2 + k_3)\}$ .

If  $W$  evolves according the spatially homogeneous kinetic equation (2.3), then

$$\begin{aligned} \frac{d}{dt} S(W) &= \int_{\mathbb{T}} dk_1 W(k_1)^{-1} C(W)(k_1) \\ &= 12\pi \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4 = \pm 1} \int_{\mathbb{T}^4} dk_1 dk_2 dk_3 dk_4 (16\omega_1 \omega_2 \omega_3 \omega_4)^{-1} \delta\left(\sum_{j=1}^4 \sigma_j \omega_j\right) \delta\left(\sum_{j=1}^4 \sigma_j k_j\right) \\ &\quad \times W_1^{-1} \sigma_1 (\sigma_1 W_2 W_3 W_4 + W_1 \sigma_2 W_3 W_4 + W_1 W_2 \sigma_3 W_4 + W_1 W_2 W_3 \sigma_4) \\ &= 3\pi \sum_{\sigma_1, \sigma_2, \sigma_3, \sigma_4 = \pm 1} \int_{\mathbb{T}^4} dk_1 dk_2 dk_3 dk_4 (16\omega_1 \omega_2 \omega_3 \omega_4)^{-1} \delta\left(\sum_{j=1}^4 \sigma_j \omega_j\right) \delta\left(\sum_{j=1}^4 \sigma_j k_j\right) \\ &\quad \times W_1 W_2 W_3 W_4 \left(\sum_{j=1}^4 \sigma_j W_j^{-1}\right)^2. \end{aligned} \quad (3.13)$$

We conclude that the entropy production is non-negative and that  $dS(W)/dt = 0$  if and only if  $1/W$  is a positive collisional invariant.

Vice versa, if  $\psi$  is a collisional invariant and  $\psi(k) \geq 0$ , then setting  $W(k) = 1/\psi(k)$  one has

$$C(W)(k) = 0. \quad (3.14)$$

Thus stationary solutions are uniquely characterized by  $1/W$  being a positive collisional invariant. In brackets we remark that a complete discussion would have to specify in which function space one searches for collisional invariants.

Collisional invariants are studied in [29], where the following result is proved.  $\omega$  is assumed to have no flat pieces in the sense that the set  $\{k \in \mathbb{T}^3 \mid \det \text{Hess} \omega(k) = 0\}$  has at most the dimension two. Here Hess is the Hessian of  $\omega$  as a  $3 \times 3$  matrix. Let  $\psi : \mathbb{T}^3 \rightarrow \mathbb{R}$  be measurable,  $\int_{\mathbb{T}^3} dk |\psi(k)| < \infty$ , and a collisional invariant under pair collisions, in the sense that (3.11) holds Lebesgue almost surely. Then  $\psi$  is necessarily of the form

$$\psi(k) = a + c\omega(k) \quad (3.15)$$

with some constants  $a, c \in \mathbb{R}$ . By our previous discussion this implies that the kinetic equation has a two-parameter family of stationary solutions. If (3.15) is inserted in the

3-phonons merger (3.12), then  $a = 0$  necessarily. To have thermal equilibrium as only stationary solutions, there must be 3-phonons mergers on a set of full dimension. A more physical mechanism would be to include a cubic on-site potential, which appears naturally in an expansion with respect to the anharmonicity, unless there are special symmetries which would make this order to vanish. For the cubic potential a collisional invariant must satisfy the 2-phonons merger condition, which is (3.12) upon dropping  $k_3$ . Again, if there is a set of full dimension of 2-phonons mergers, then the only stationary solutions are the ones corresponding to thermal equilibrium.

Our discussion has interesting implications on the very widely studied Fermi-Pasta-Ulam problem [30], see the special issue [31] at the occasion of its 50-th anniversary. Fermi, Pasta, and Ulam considered chains of anharmonic oscillators and studied by a numerical iteration scheme the relaxation to equipartition, i.e. to thermal equilibrium. To their surprise, such an approach did not take place, at least not on the time scale of the computation. One explanation comes from the KAM theory which demonstrates that in part the invariant tori of the linear dynamics persist under small nonlinear perturbations. Thus a Lebesgue typical phase point may not explore the full energy shell. A second explanation relies on the fact that for a special choice of the nonlinearity the Hamiltonian system remains integrable and admits propagating soliton solutions. Also, for the FPU model there are special solutions, the breathers, which may impede the relaxation to thermal equilibrium.

Kinetic theory operates in a different part of phase space. The energy is proportional to the length of the chain and the nonlinearity is weak. In this regime the phonon picture is precise. Propagation is encoded by the dispersion relation  $\omega$ , while the relaxation comes from the phonon collisions. For the FPU chain one has  $\omega(k) = (1 - \cos(2\pi k))^{1/2}$ ,  $k \in \mathbb{T}$ . Thus, ignoring special  $k$ -values, phonons propagate ballistically with non-zero speed. On the other hand, the collision rule depends on the precise form of the nonlinearity. For the FPU  $\alpha$ -chain the couplings are cubic as  $(q_{j+1} - q_j)^3$ . In this case the collision term vanishes which signals poor relaxation. For the FPU  $\beta$ -chain the couplings are quartic as  $(q_{j+1} - q_j)^4$ . A detailed analysis shows that the energy current correlation, as based on kinetic theory, has a slow decay as  $t^{-3/5}$  [27, 33], a result with good numerical support [32]. If instead one chooses as nonlinearity a quartic on-site potential, as  $q_j^4$ , then the energy current correlation decays exponentially [28]. In this case kinetic theory predicts a rapid convergence to equilibrium, as is well confirmed by molecular dynamics simulations [28, 34], also away from the limiting kinetic regime.

## 4 References

- [1] N. Brilliantov and T. Pöschel, *Kinetic Theory of Granular Gases*, Oxford University Press 2004.
- [2] H. Grad, *Principles of the Kinetic Theory of Gases*. Handbuch der Physik, Band 12, pp. 205–294. Springer, Berlin, Heidelberg, 1958.
- [3] O.E. Lanford, *Time Evolution of Large Classical Systems*, ed. J. Moser, *Lecture Notes in Physics* Vol. 38, pp. 1–111, Springer, Heidelberg, 1975.
- [4] C. Cercignani, R. Illner, and M. Pulvirenti, *The Mathematical Theory Of Dilute Gases*, Springer, Berlin, 1994.

- [5] H. Spohn, Large Scale Dynamics of Interacting Particles, Texts and Monographs in Physics, Springer Verlag, Heidelberg, 1991.
- [6] L.W. Nordheim, On the kinetic method in the new statistics and its application in the electron theory of conductivity, Proc. Roy. Soc. **119**, 689–698 (1929).
- [7] R.E. Peierls, Zur kinetischen Theorie der Wärmeleitung in Kristallen, Annalen Physik **3**, 1055–1101 (1929).
- [8] E.A. Uehling and G.E. Uhlenbeck, Transport phenomena in Einstein-Bose and Fermi-Dirac gases, Phys. Rev. **43**, 552–561 (1933).
- [9] L. Erdős, M. Salmhofer, and H.T. Yau, On the quantum Boltzmann equation, J. Stat. Phys. **116**, 367–380 (2004).
- [10] D. Benedetto, F. Castella, R. Esposito, and M. Pulvirenti, Some considerations on the derivation of the nonlinear quantum Boltzmann equation, J. Stat. Phys. **116**, 381–410 (2004).
- [11] H. Spohn, Kinetic Equations for Quantum Many-Particle Systems, Modern Encyclopedia of Mathematical Physics, to appear.
- [12] G. Leibfried, Gittertheorie der mechanischen und thermischen Eigenschaften der Kristalle, Handbuch der Physik Band VII/1, Kristallphysik, ed. S. Flügge, Springer, Berlin 1955.
- [13] J. M. Ziman, Electrons and Phonons, Clarendon Press, Oxford, 1960.
- [14] V.L. Gurevich, Transport in Phonon Systems, North-Holland 1986.
- [15] G. Eyink and H. Spohn, Space-time invariant states of the ideal gas with finite number, energy, and entropy density, in: On Dobrushin’s Way. From Probability Theory to Statistical Physics, eds. R. Minlos, S. Shlosman, Y. Suchov, Advances in the Mathematical Sciences, Ser. 2, Vol. 198, pp. 71–89, AMS 2000.
- [16] A. Mielke, Macroscopic behavior of microscopic oscillations in harmonic lattices via Wigner-Husimi transforms, Arch. Ration. Mech. Anal. **118**, 401–448 (2006).
- [17] L. Harris, J. Lukkarinen, S. Teufel, and F. Theil, Energy transport by acoustic modes of harmonic lattices, arXiv:math-ph/0611052.
- [18] T. Dudnikova and H. Spohn, Local stationarity for lattice dynamics in the harmonic approximation, Markov Processes and Related Fields, **12**, 645–678 (2006).
- [19] H. Spohn, The phonon Boltzmann equation, properties and link to weakly anharmonic lattice dynamics, J. Stat. Phys. **124**, 1041–1104 (2006).
- [20] V.E. Zakharov, V.S. L’vov, and G. Falkovich, Kolmogorov Spectra of Turbulence: I Wave Turbulence. Springer, Berlin, 1992.
- [21] P. Janssen, The Interaction of Waves and Wind, Cambridge University Press 2004.
- [22] Y. Choi, Y.V. Lvov, and S. Nazarenko, Joint statistics of amplitudes and phases in wave turbulence, Physica **D 201**, 121–149 (2005).
- [23] H. Spohn, Towards a microscopic derivation of the phonon Boltzmann equation, in: Mathematical Physics of Quantum Mechanics, eds. J. Asch, A. Joye, Lecture Notes in Physics Vol. 690, pp. 295–304, Springer, Berlin, 2006.
- [24] N.T. Ho and L.J. Landau, Fermi gas on a lattice in the van Hove limit, J. Stat. Phys. **87**, 821–845 (1997).
- [25] D. Benedetto, F. Castella, R. Esposito, and M. Pulvirenti, On the weak coupling limit for bosons and fermions, Math. Mod. Meth. Appl. Sci. **15**, 1811–1843 (2005).

- [26] D. Benedetto, F. Castella, R. Esposito, and M. Pulvirenti, From the  $N$ -body Schrödinger equation to the quantum Boltzmann equation: a term-by-term convergence result in the weak coupling regime, preprint.
- [27] A. Pereverzev, Fermi-Pasta-Ulam  $\beta$  lattice: Peierls equation and anomalous heat conductivity, Phys. Rev. E **68**, 056 (2003).
- [28] S. Aoki, J. Lukkarinen, and H. Spohn, Energy transport in weakly anharmonic chains, J. Stat. Phys. **124**, 1105–1129 (2006).
- [29] H. Spohn, Collisional invariants for the phonon Boltzmann equation, J. Stat. Phys. **124**, 1131–1135, (2006).
- [30] E. Fermi, J. Pasta, and S. Ulam, Studies in nonlinear problems, I, in Nonlinear Wave Motion, A.C. Newell, ed. (American Mathematical Society, Providence, RI, 1974), pp. 143–156. Originally published as Los Alamos Report LA-1940 in 1955.
- [31] Focus Issue: The “Fermi-Pasta-Ulam” problem – the first 50 years, Chaos **15** (1), (2005).
- [32] S. Lepri, R. Livi, and A. Politi, Thermal conductivity in classical low-dimensional lattices, Physics Reports **377**, 1–80 (2003).
- [33] J. Lukkarinen and H. Spohn, Kinetic theory of FPU chains, in preparation.
- [34] K. Aoki and D. Kusnezov, Nonequilibrium statistical mechanics of classical lattice  $\phi^4$  field theory, Ann. Phys. **295**, 50–80 (2002).

Herbert Spohn  
Zentrum Mathematik and Physik Department, TU München,  
Boltzmannstr. 3, D-85747 Garching, Germany

E-mail: spohn@ma.tum.de